

Scaling of solvation force in 2D Ising strip

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The solvation force for the 2D Ising strip is calculated via exact diagonalization of the transfer matrix in two cases: the symmetric case corresponds to identical surface fields, and the antisymmetric case to exactly opposite surface fields. In the symmetric case the solvation force is always negative (attractive) while in the antisymmetric case the solvation force is positive (repulsive) at high temperatures and negative at low temperatures. It changes sign close to the critical wetting temperature characterizing the semi-infinite system. The properties of the solvation force are discussed and the scaling function describing its dependence on temperature, surface field, and strip's width is proposed.

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I. INTRODUCTION

Properties of the solvation force in various condensed matter systems have been the subject of very intensive research during recent years [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]. Lattice models play special role among considered systems. Although many important results were obtained in this field by different methods of taking into account fluctuations which determine the properties of the analyzed systems, the approach based on the exact evaluation of the partition function via the transfer matrix method still plays a distinguished role. Below we report our results on the properties of the solvation force for 2D Ising strip. They are obtained via exact diagonalization of the transfer matrix which is then followed by numerical solutions of equations for eigenvalues.

We consider Ising model on a two-dimensional square lattice consisting of M rows and N columns. There is no bulk magnetic field acting on the system and there are two surface fields: h_1 acts on spins in the first row and h_2 acts on the M -th row. The Hamiltonian of this model takes the standard form

$$\begin{aligned} \mathcal{H}(\{s_i\}) = & -J \sum_{n=1}^N \sum_{m=1}^{M-1} s_{n,m} s_{n,m+1} \\ & -J \sum_{n=1}^N \sum_{m=1}^M s_{n,m} s_{n+1,m} \\ & -h_1 \sum_{n=1}^N s_{n,1} - h_2 \sum_{n=1}^N s_{n,M}, \end{aligned} \quad (1)$$

where $s_{n,m} = \pm 1$ with $n = 1, \dots, N$, $m = 1, \dots, M$ denotes the spin located in the n -th column and m -th row, and J is the coupling constant. Periodic boundary conditions in the horizontal direction are imposed: $s_{N+1,m} \equiv s_{1,m}$.

Our purpose is to determine the properties of the solvation force experienced by the system boundaries. In the following we consider two cases: the symmetric case (S) corresponds to $h_1 = h_2$, and for the antisymmetric case (AS) one has $h_1 = -h_2$.

Although the strip of finite width experiences no phase transition, we shall often refer to two critical temperatures: the bulk critical temperature $k_B T_c = 2J / \ln(1 + \sqrt{2})$, and the wetting temperature T_w which characterizes the critical wetting transition in a semi-infinite system with surface field h_1 . The wetting temperature fulfills the equation

$$\cosh 2K_1 = \cosh 2K - \sinh 2K e^{-2K}, \quad (2)$$

where $K = J / (k_B T_w)$, $K_1 = h_1 / (k_B T_w)$, and k_B is the Boltzmann constant. For a small surface field h_1 this equation leads to

$$\frac{T_c - T_w}{T_c} = \frac{1}{4} (1 + \sqrt{2}) \ln(1 + \sqrt{2}) \left(\frac{h_1}{J} \right)^2, \quad \frac{h_1}{J} \rightarrow 0. \quad (3)$$

For $h_1 \geq J$ one has $T_w = 0$ and there is no wetting transition.

II. SOLVATION FORCE

The dimensionless free energy per one column is defined as

$$f(T, h_1, M) = \lim_{N \rightarrow \infty} \frac{1}{N} \frac{\mathcal{F}}{k_B T} = - \lim_{N \rightarrow \infty} \frac{\ln \mathcal{Z}}{N}, \quad (4)$$

where \mathcal{Z} is the canonical partition function for the Hamiltonian (1) which we evaluate using the exact transfer matrix method [11, 12]. The free energy may be separated into three types of contributions

$$f(T, h_1, M) = M f_b(T) + f_s(T, h_1) + f_{\text{int}}(T, h_1, M), \quad (5)$$

where f_b is the bulk free energy per one spin [13] and f_s is the surface free energy; both f_b and f_s are M -independent. The remaining term f_{int} describes the interaction between the system boundaries. It tends to 0

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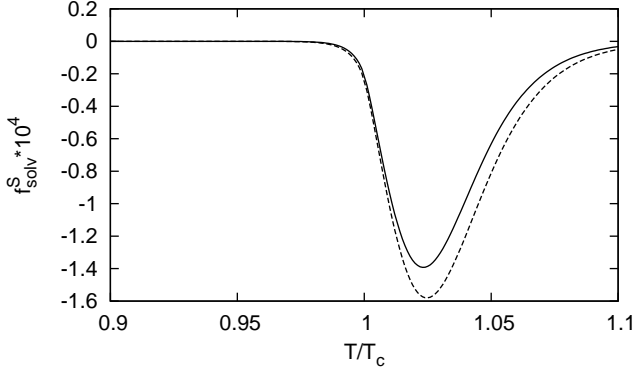


FIG. 1: Comparison of the solvation force f_{solv}^S for $T_w = 0.8T_c$ ($h_1 \approx 0.60J$) (solid curve) and $T_w = 0$ ($h_1 = J$) (broken curve) for symmetric case $h_1 = h_2$. Both curves correspond to the value $M = 50$.

as M goes to infinity and from this term the solvation force originates.

The solvation force is, in general, defined as the minus derivative of f_{int} wrt M . In our case, because M takes only integer values, we use the definition

$$f_{\text{solv}}(T, h_1, M) = -[f_{\text{int}}(T, h_1, M+1) - f_{\text{int}}(T, h_1, M)], \quad (6)$$

which leads to the following expression

$$f_{\text{solv}}(T, h_1, M) = f(T, h_1, M) - f(T, h_1, M+1) - f_b. \quad (7)$$

The solvation force for the 2D strip has been already analyzed in the $T_w = 0$ case [5] corresponding to $h_1 = J$. Our analysis covers the whole spectrum $T_w \geq 0$, i.e. $h_1 \leq J$. To calculate the solvation force we used the methods described in [11, 12, 14, 15]. The complete analysis (including also the inhomogeneous boundary fields) will be published elsewhere [16]; here we discuss only the main results.

First we briefly discuss the symmetric case (S). The corresponding solvation force f_{solv}^S is plotted in Fig.1 for two cases: $T_w > 0$ (solid curve) and $T_w = 0$ (broken curve). The difference between these two functions is only of quantitative nature — decreasing the surface field h_1 , i.e. increasing the wetting temperature T_w results in decreasing the absolute value of the solvation force. The minimum of the solvation force f_{solv}^S is located at $T_{\text{min}}^S > T_c$.

For opposite surface fields (AS) the solvation force $f_{\text{solv}}^{\text{AS}}$ in the $T_w > 0$ case, i.e., $h_1 < J$, differs substantially from the $T_w = 0$, i.e., $h_1 = J$ case. Fig.2 presents a typical plot of $f_{\text{solv}}^{\text{AS}}$ as a function of T . For low temperatures this force is negative (attractive) and has a minimum at $T_{\text{min}}^{\text{AS}} < T_w$. The solvation force is negative at wetting temperature and has a zero at $T^* > T_w$. Above T^* the solvation force is positive (repulsive) and has a maximum at $T_{\text{max}}^{\text{AS}} < T_c$ (for M large enough). This remains in contrast with the $T_w = 0$ case in which the solvation force is positive for all temperatures.

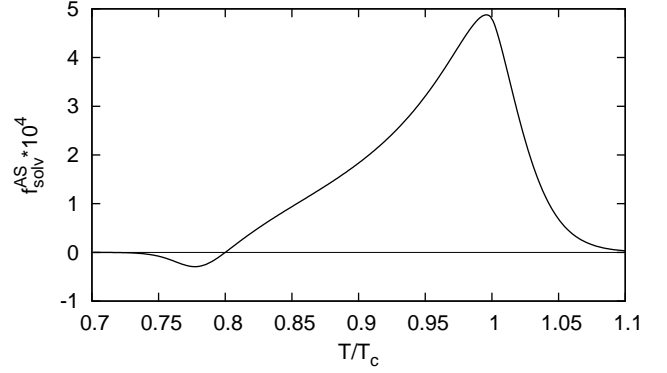


FIG. 2: The solvation force $f_{\text{solv}}^{\text{AS}}$ as a function of temperature for $T_w = 0.8T_c$ (i.e. $h_1 \approx 0.60J$) and $M = 50$ in the antisymmetric case $h_1 = -h_2$. Note that the difference between the zero of the solvation force T^* and the wetting temperature T_w is not visible in this scale.

Exactly at the bulk critical temperature T_c the dependence of the solvation force on M has been found using conformal invariance [17, 18]

$$f_{\text{solv}}^S(T_c, h_1, M) = -\frac{\pi}{48M^2} + \mathcal{O}(1/M^3), \quad (8)$$

$$f_{\text{solv}}^{\text{AS}}(T_c, h_1, M) = \frac{23\pi}{48M^2} + \mathcal{O}(1/M^3). \quad (9)$$

This result, in particular the universal values of the amplitudes, has been reproduced by our analysis.

In the rest of this paper we exclusively discuss the antisymmetric case (AS).

First we concentrate on the temperature T^* at which the solvation force becomes zero. We have found that for fixed $h_1 > 0$ and for $M \rightarrow \infty$ this temperature approaches the wetting temperature T_w exponentially

$$\frac{T^* - T_w}{T_c} = A(h_1) e^{-B(h_1)M}, \quad M \rightarrow \infty, \quad (10)$$

where $A(h_1)$ and $B(h_1)$ are positive functions of the surface field h_1 [21]. We have found that for $h_1 \rightarrow 0$, i.e., $T_w \rightarrow T_c$ one has

$$\lim_{h_1 \rightarrow 0} A(h_1) = 0. \quad (11)$$

We note that this result is different from the corresponding result obtained within the mean field theory where T^* is exponentially shifted *below* T_w . It is also different from the corresponding result obtained for the restricted solid-on-solid (RSOS) model, where T^* is *equal* to T_w [19].

III. SCALING FUNCTION

In this section we discuss the scaling function that describes the behavior of the solvation force $f_{\text{solv}}^{\text{AS}}(T, h_1, M)$ for large M and subcritical temperatures. The relevant

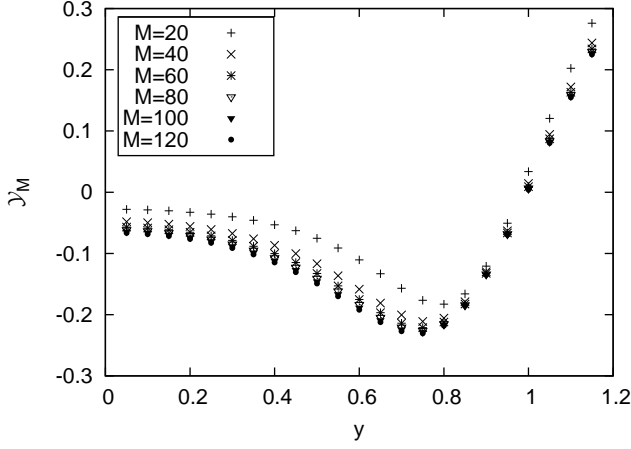


FIG. 3: Convergence of the scaling function. The function \mathcal{Y}_M is evaluated for $x = 1$ and for several values of y and M presented on the plot.

scaling function $\mathcal{X}(x)$ has already been proposed to describe $f_{\text{solv}}^{\text{AS}}$ in the $T_w = 0$ case [5]

$$f_{\text{solv}}^{\text{AS}}(T, h_1 = J, M) = \frac{1}{M^2} \mathcal{X}\left(\frac{M}{\xi^-(T)}\right). \quad (12)$$

The correlation length for 2D Ising model close to T_c is $\xi^-(T) = \xi_0^- t^{-1}$, where $t = (T_c - T)/T_c > 0$ and $\xi_0^- = [4 \ln(1 + \sqrt{2})]^{-1}$. The scaling function $\mathcal{X}(x)$ can be obtained numerically from the transfer matrix spectrum and some of its properties can be proved analytically (see Eq.(9) and [20]), namely

$$\mathcal{X}(0) = 23\pi/48, \quad (13)$$

$$\mathcal{X}(x) = 2\pi^2/x, \quad \text{for } x \rightarrow \infty. \quad (14)$$

Here we would like to extend this result to $h_1 < J$, i.e. $T_w > 0$ case.

For 2D Ising model the gap exponent $\Delta_1 = 1/2$ and for $T < T_c$ the following scaling behavior

$$f_{\text{solv}}^{\text{AS}}(T, h_1, M) = \frac{1}{M^2} \mathcal{Y}(x, y), \quad (15)$$

where

$$x = \frac{M}{\xi_0^- t^{-1}}, \quad y = \frac{A_0}{k_B T_c} \frac{h_1}{t^{1/2}} \quad (16)$$

comes into play in the limit $M \rightarrow \infty$ with x and y fixed. This implies additionally the $t \rightarrow 0$, $h_1 \rightarrow 0$ and $T_w \rightarrow T_c$ limits. The coefficient $A_0 = [(1 + \sqrt{2}) / \ln(1 + \sqrt{2})]^{1/2}$ in Eq.(16) has been introduced such that the value $y = 1$ corresponds to $T = T_w$ and then Eq.(3) is satisfied. For $y < 1$ Eq.(15) gives the solvation force $f_{\text{solv}}^{\text{AS}}$ below the wetting temperature and for $y > 1$ above T_w .

Eq.(15) may be rewritten in the form leading to the scaling function

$$\mathcal{Y}(x, y) = \lim_{M \rightarrow \infty} \mathcal{Y}_M(x, y), \quad (17)$$

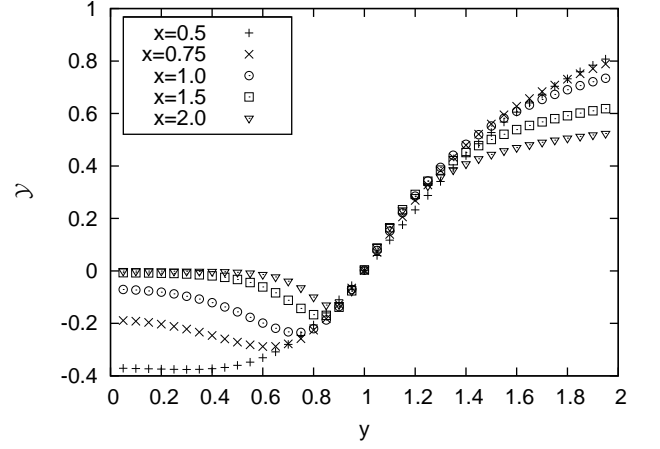


FIG. 4: Plots of the scaling function \mathcal{Y} . All plots were obtained from \mathcal{Y}_M for $M = 200$.

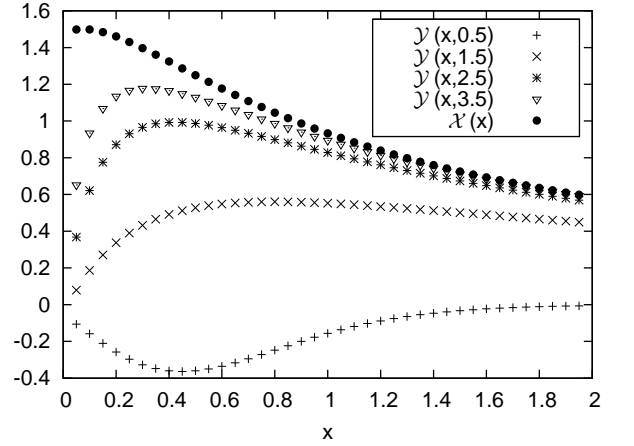


FIG. 5: The scaling function \mathcal{Y} plotted for $y = 0.5, 1.5, 2.5, 3.5$ and the scaling function \mathcal{X} . All points were calculated for $M = 200$.

where

$$\mathcal{Y}_M(x, y) = \quad (18)$$

$$M^2 f_{\text{solv}} \left(T_c \left(1 - \frac{x \xi_0^-}{M} \right), k_B T_c y \left(\frac{M}{x \xi_0^- A_0^2} \right)^{1/2}, M \right).$$

Fig.3 presents plots of \mathcal{Y}_M for fixed value of $x = 1$ and selected values of $y \in [0, 1.2]$ to exhibit the convergence of the series \mathcal{Y}_M . Typically, for M large enough one has

$$\mathcal{Y}_M(x, y) = \mathcal{Y}(x, y) + \frac{C(x, y)}{M} + O(M^{-2}). \quad (19)$$

To estimate the values of the function \mathcal{Y} we evaluated \mathcal{Y}_M for $M = 200$. We note that a different way of obtaining the function \mathcal{Y} , based on the least squares method which allows to calculate the functions \mathcal{Y} and C in Eq.(19), leads to similar results (the differences are not visible on the scale of our figures). The plots of function \mathcal{Y} are shown on Fig.4.

Next we investigate the relation between the scaling functions $\mathcal{Y}(x, y)$ and $\mathcal{X}(x)$. The function $\mathcal{X}(x)$ is calculated in the limit $M \rightarrow \infty, t \rightarrow 0$ with h_1 and Mt fixed. By applying this limit to Eqs (15) and (12) one gets

$$\mathcal{X}(x) = \lim_{y \rightarrow \infty} \mathcal{Y}(x, y). \quad (20)$$

The functions $\mathcal{X}(x)$ and $\mathcal{Y}(x, y)$ plotted for selected values of y are presented on Fig.5. Additionally we have found that $\mathcal{X}(x) - \mathcal{Y}(x, y) \propto y^{-2}$ for large y .

The scaling function $\mathcal{Y}(x, y)$ changes its sign, see Figs 4, 5. The zeros of the scaling function are denoted by $y^*(x)$, i.e., $\mathcal{Y}(x, y^*(x)) = 0$. We have found that for large x the function $y^*(x)$ approaches 1 exponentially from above. This allows us to show that in the scaling limit $M \rightarrow \infty, h_1 \rightarrow 0$, and Mh_1^2 fixed one has

$$\begin{aligned} \frac{T^* - T_w}{T_c} &= \frac{T_c - T_w}{T_c} - \frac{1}{M} f\left(\frac{Mh_1^2}{k_B^2 T_c^2}\right) + \mathcal{O}(1/M^2), \\ &= \frac{1}{M} g\left(\frac{Mh_1^2}{k_B^2 T_c^2}\right) + \mathcal{O}(1/M^2), \end{aligned} \quad (21)$$

where $f(\zeta)$ and $g(\zeta)$ are positive functions which can be determined via an implicit formula

$$A_0 \zeta^{1/2} = [f(\zeta)]^{1/2} y^*(f(\zeta)/\xi_0^-), \quad (22)$$

$$g(\zeta) = A_0^2 - f(\zeta). \quad (23)$$

We note that Eq.(21) is different from Eq.(10) because different limiting procedures were applied in these two cases.

IV. CONCLUSIONS

In the symmetric case of identical surface fields the solvation force is negative (attractive) and has minimum at supercritical temperature. The solvation force calculated for system parameters such that $T_w > 0$ differs only quantitatively from the one in case $T_w = 0$, see Fig.1.

In the antisymmetric case of opposite surface fields the solvation force is positive at high temperatures and negative at low temperatures; it changes its sign at temperature $T^* > T_w$, see Fig.2. In the case h_1 fixed and $M \rightarrow \infty$ the difference $T^* - T_w$ approaches 0 exponentially quickly in M .

The scaling function $\mathcal{Y}(x, y)$ was proposed to describe the behavior of the solvation force for $T < T_c$ in the limit $h_1 \rightarrow 0$ and $M \rightarrow \infty$, see Figs 4, 5. We checked that in the limit of high surface field ($y \rightarrow \infty$ in Eq.(15)) this scaling function approached the scaling function describing the scaling behavior of the solvation force in the $T_w = 0$ case. In addition, the zeros of the scaling function were investigated to find the formula for $T^* - T_w$ in the $h_1 \rightarrow 0$ limit.

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 - [21] In principle, these functions can be found by fitting Eq.(10) to our numerical results. However, for $T_w > 0.5T_c$ and for $M \geq 10$ the difference between T^* and T_w is of order of numerical errors and we were unable to precisely determine the functions $A(h_1)$ and $B(h_1)$.